



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2016 – 06:08 PM EDT

PDB ID : 5III
Title : Crystal structure of the pre-catalytic ternary complex of DNA polymerase lambda with a templating 8-oxo-dG and an incoming dATP
Authors : Burak, M.J.; Guja, K.E.; Garcia-Diaz, M.
Deposited on : 2016-03-01
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

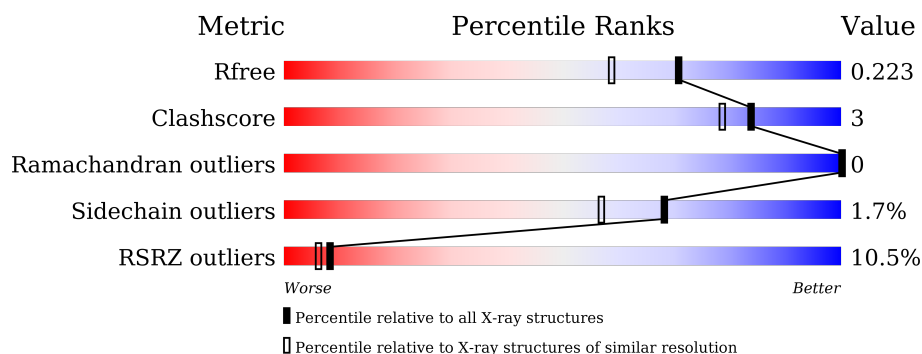
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div>10%</div> <div> <div></div> <div>89%</div> <div>5% • 6%</div> </div> </div>
2	D	4	<div> <div>75%</div> <div>25%</div> </div>
3	P	6	<div> <div>100%</div> </div>
4	T	11	<div> <div>82%</div> <div>9% 9%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3173 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2381	1506	425	439	11			

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

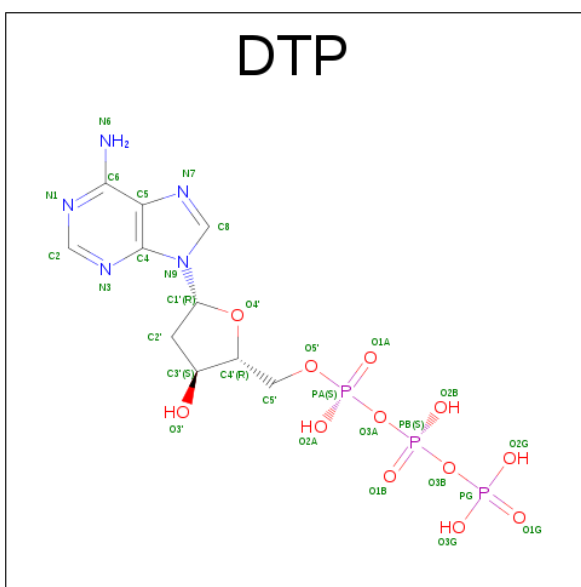
- Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*GP*TP*AP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	6	Total	C	N	O	P	0	0	0
			118	58	23	32	5			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*GP*CP*(8OG)P*GP*TP*AP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	11	Total	C	N	O	P	0	0	0
			226	107	43	66	10			

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	0
			2	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

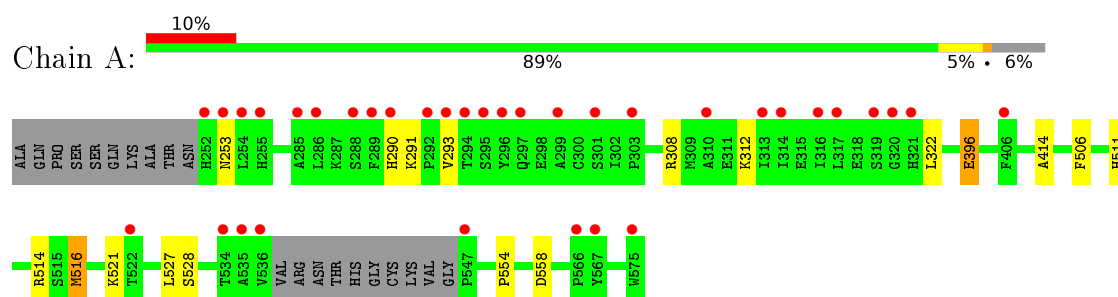
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	243	Total	O	0	0
			243	243		
8	D	3	Total	O	0	0
			3	3		
8	P	28	Total	O	0	0
			28	28		
8	T	58	Total	O	0	0
			58	58		

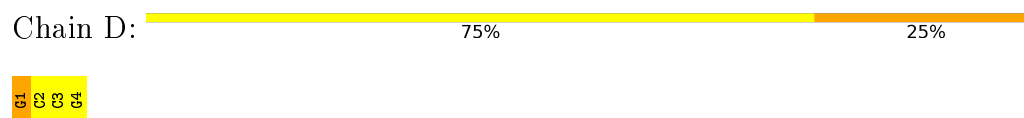
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA polymerase lambda



- Molecule 2: DNA (5'-D(P*GP*CP*CP*G)-3')

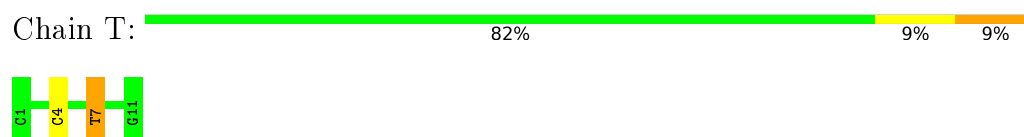


- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*AP*(DOC))-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(*CP*GP*GP*CP*(8OG)P*GP*TP*AP*CP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.85Å 62.68Å 140.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.70 – 1.80 41.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.70-1.80) 93.8 (41.70-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.201 , 0.225 0.199 , 0.223	Depositor DCC
R_{free} test set	2109 reflections (4.85%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3173	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, DTP, DOC, 8OG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/2431	0.48	0/3295
2	D	1.27	1/92 (1.1%)	0.83	0/138
3	P	0.79	0/112	0.95	0/171
4	T	0.82	0/226	1.17	3/345 (0.9%)
All	All	0.47	1/2861 (0.0%)	0.61	3/3949 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	DG	OP3-P	-10.34	1.48	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	7	DT	C1'-O4'-C4'	-5.61	104.49	110.10
4	T	7	DT	O5'-P-OP2	-5.50	100.75	105.70
4	T	7	DT	O4'-C4'-C3'	-5.06	102.48	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2381	0	2285	13	0
2	D	83	0	45	3	0
3	P	118	0	69	0	0
4	T	226	0	125	2	0
5	A	30	0	12	1	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	243	0	0	2	0
8	D	3	0	0	0	0
8	P	28	0	0	0	0
8	T	58	0	0	0	0
All	All	3173	0	2536	16	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLU:HG3	1:A:414:ALA:HB2	1.75	0.69
5:A:601:DTP:O2G	8:A:701:HOH:O	2.11	0.68
1:A:308:ARG:NH2	2:D:1:DG:OP2	2.33	0.62
1:A:253:ASN:N	1:A:253:ASN:OD1	2.39	0.56
1:A:290:HIS:HE1	1:A:291:LYS:HE2	1.72	0.55
1:A:521:LYS:NZ	4:T:4:DC:OP1	2.35	0.54
2:D:3:DC:H2'	2:D:4:DG:C8	2.44	0.53
2:D:2:DC:H2'	2:D:3:DC:C6	2.45	0.52
1:A:396:GLU:OE1	8:A:702:HOH:O	2.19	0.50
1:A:312:LYS:HG3	1:A:322:LEU:HD11	1.95	0.48
1:A:308:ARG:O	1:A:312:LYS:HD3	2.14	0.47
1:A:511:HIS:CE1	1:A:514:ARG:HH21	2.34	0.46
1:A:516:MET:HG2	1:A:527:LEU:CD2	2.45	0.46
1:A:290:HIS:CE1	1:A:291:LYS:HE2	2.52	0.43
1:A:528:SER:HB2	4:T:7:DT:H5'	2.02	0.41
1:A:554:PRO:HG2	1:A:558:ASP:OD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/334 (93%)	300 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/280 (84%)	232 (98%)	4 (2%)	68	57

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	VAL
1	A	396	GLU
1	A	506	PHE
1	A	516	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DOC	P	6	3,4	12,19,20	4.29	9 (75%)	14,26,29	2.18	2 (14%)
4	8OG	T	5	4	16,25,26	5.18	10 (62%)	20,37,40	2.58	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DOC	P	6	3,4	-	0/3/18/19	0/2/2/2
4	8OG	T	5	4	-	0/3/21/22	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	5	8OG	C3'-C4'	-7.97	1.30	1.53
3	P	6	DOC	C3'-C2'	-7.63	1.32	1.54
3	P	6	DOC	O4'-C4'	-6.70	1.29	1.44
4	T	5	8OG	O4'-C1'	-4.20	1.32	1.42
3	P	6	DOC	C4-N4	2.27	1.41	1.35
3	P	6	DOC	C5-C4	2.41	1.46	1.41
4	T	5	8OG	O3'-C3'	2.65	1.49	1.43
3	P	6	DOC	C4-N3	3.23	1.41	1.35
4	T	5	8OG	C2-N2	3.64	1.41	1.34
4	T	5	8OG	C6-C5	3.79	1.49	1.41
3	P	6	DOC	C2-N3	3.90	1.46	1.38
3	P	6	DOC	C6-C5	3.99	1.46	1.38
4	T	5	8OG	C2-N1	4.80	1.44	1.35
4	T	5	8OG	C6-N1	5.00	1.42	1.33
4	T	5	8OG	C4-N3	5.10	1.43	1.35
3	P	6	DOC	C6-N1	5.35	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	6	DOC	O4'-C1'	5.63	1.55	1.42
4	T	5	8OG	O4'-C4'	7.61	1.62	1.45
4	T	5	8OG	C8-N7	13.27	1.48	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	5	8OG	O4'-C1'-N9	-8.06	101.29	108.16
4	T	5	8OG	N3-C2-N1	-5.40	120.22	127.56
4	T	5	8OG	C5-C6-N1	-3.31	119.19	123.52
3	P	6	DOC	C3'-C2'-C1'	2.46	105.54	102.75
4	T	5	8OG	C6-N1-C2	3.58	120.08	115.88
3	P	6	DOC	C6-C5-C4	6.60	120.02	117.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DTP	A	601	7	25,32,32	2.98	10 (40%)	26,50,50	2.80	4 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DTP	A	601	7	-	0/18/34/34	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	DTP	C2'-C3'	-10.28	1.25	1.52
5	A	601	DTP	O4'-C4'	-6.66	1.29	1.45
5	A	601	DTP	C5-C4	-2.19	1.35	1.40
5	A	601	DTP	C2'-C1'	2.03	1.58	1.52
5	A	601	DTP	C6-N6	2.07	1.42	1.34
5	A	601	DTP	C2-N1	2.14	1.38	1.33
5	A	601	DTP	C2-N3	2.82	1.37	1.32
5	A	601	DTP	O3'-C3'	2.97	1.50	1.43
5	A	601	DTP	O4'-C1'	3.38	1.50	1.42
5	A	601	DTP	C3'-C4'	4.23	1.65	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	DTP	N3-C2-N1	-11.83	119.58	128.87
5	A	601	DTP	N6-C6-N1	-6.22	108.08	118.52
5	A	601	DTP	C1'-N9-C4	-2.83	122.94	127.07
5	A	601	DTP	O4'-C1'-N9	2.26	111.66	107.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	DTP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/334 (94%)	0.39	35 (11%) 7 5	18, 31, 65, 82	0
2	D	4/4 (100%)	-0.49	0 100 100	35, 35, 36, 38	0
3	P	5/6 (83%)	-0.30	0 100 100	19, 19, 21, 21	0
4	T	10/11 (90%)	-0.42	0 100 100	21, 25, 37, 39	0
All	All	333/355 (93%)	0.35	35 (10%) 8 6	18, 31, 64, 82	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	VAL	7.4
1	A	535	ALA	7.0
1	A	289	PHE	5.7
1	A	547	PRO	5.5
1	A	534	THR	4.6
1	A	252	HIS	4.6
1	A	406	PHE	4.5
1	A	254	LEU	4.4
1	A	317	LEU	4.1
1	A	253	ASN	4.0
1	A	255	HIS	3.9
1	A	299	ALA	3.8
1	A	290	HIS	3.7
1	A	319	SER	3.6
1	A	294	THR	3.6
1	A	301	SER	3.3
1	A	316	ILE	3.1
1	A	297	GLN	3.0
1	A	313	ILE	2.9
1	A	288	SER	2.8
1	A	296	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	567	TYR	2.7
1	A	575	TRP	2.6
1	A	292	PRO	2.6
1	A	522	THR	2.6
1	A	314	ILE	2.6
1	A	321	HIS	2.4
1	A	536	VAL	2.4
1	A	286	LEU	2.3
1	A	320	GLY	2.2
1	A	566	PRO	2.2
1	A	295	SER	2.1
1	A	303	PRO	2.1
1	A	285	ALA	2.1
1	A	310	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	8OG	T	5	23/24	0.93	0.11	-	23,27,43,47	0
3	DOC	P	6	18/19	0.98	0.14	-	18,21,24,27	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DTP	A	601	30/30	0.98	0.12	0.26	19,22,25,27	0
6	NA	A	602	1/1	0.99	0.07	-5.70	19,19,19,19	0
7	MG	A	604	1/1	0.99	0.13	-	21,21,21,21	0
6	NA	A	603	1/1	0.97	0.07	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.